Projective Space Method for Slow Invariant Manifolds of Reactive Systems

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Introduction

Motivation and background

- Detailed kinetics are essential for accurate modeling of real systems.
- Reactive flow systems admit multi-scale solutions.
- Manifold methods provide a potential for computational saving.
- Slow invariant manifolds (SIMs) describe the asymptotic structure of reactive systems’ invariant attracting trajectories.
- Current manifold construction methods either approximate the actual SIMs or require a close initial guess.
Long-term objective

Create an efficient algorithm that reduces the computational cost for simulating reactive flows based on a reduction in the stiffness and dimension of the composition phase space.

Immediate objective

Construct 1-D SIMs for dynamical systems arising from modeling unsteady spatially homogenous closed reactive systems.
Slow Invariant Manifold (SIM)

- The composition phase space for closed spatially homogeneous reactive system:

\[
\frac{dz}{dt} = f(z), \quad z \in \mathbb{R}^3.
\]
Mathematical Model

For a mixture of mass $M$ confined in volume $V$ containing $N$ species composed of $L$ elements that undergo $J$ reversible reactions,

$$\frac{dn_i}{dt} = V \sum_{j=1}^{J} \nu_{ij} r_j, \quad i = 1, \ldots, N,$$

where,

$$r_j = A_j T^{\beta_j} \exp\left(\frac{-E_j}{\bar{R}T}\right) \left(\prod_{i=1}^{N} \left(\frac{n_i}{V}\right)^{\nu_{ij}} - \frac{1}{K_j^c} \prod_{i=1}^{N} \left(\frac{n_i}{V}\right)^{\nu_{ij}''}\right), \quad j = 1, \ldots, J,$$

$$K_j^c = \left(\frac{p^o}{\bar{R}T}\right)^{\sum_{i=1}^{N} \nu_{ij}} \exp\left(-\frac{\sum_{i=1}^{N} \bar{\mu}_i^{po} \nu_{ij}}{\bar{R}T}\right), \quad j = 1, \ldots, J.$$
System reduction

• In chemical reactions, atoms are conserved:

\[
\sum_{i=1}^{N} \phi_{li} \nu_{ij} = 0, \quad l = 1, \ldots, L, \quad j = 1, \ldots, J,
\]

\[
\sum_{i=1}^{N} \phi_{li} n_{i}^{*} = \sum_{i=1}^{N} \phi_{li} n_{i}, \quad l = 1, \ldots, L.
\]

• Solutions of the following form exist,

\[
n_{i} = n_{i}^{*} + M \sum_{k=1}^{R} D_{ik} z_{k}, \quad i = 1, \ldots, N.
\]

• The reactive system is recast as an autonomous dynamical system,

\[
\frac{dz_{k}}{dt} = f_{k} (z_{1}, \ldots, z_{R}), \quad k = 1, \ldots, R.
\]
Method of Construction

Equilibria

- The construction method is based on identifying all the equilibria, and connecting relevant ones via heteroclinic orbits.

- For isothermal reactive systems, reaction rates depend on combinations of polynomials of $z$.

- The set of equilibria of the full reaction network is complex: $z^e \in \mathbb{C}^R \mid f(z^e) = 0$.

- This set contains finite and infinite equilibria.

- The system’s equilibria can be positive dimensional continua.
**SIM construction**

- A 1-D SIM has a maximum of two branches that connect two equilibria to the unique physical critical point (a sink) tangent to its slowest mode.

- These equilibria are identified by their special dynamical character: *their eigenvalue spectrum contains only one unstable direction*.

- Heteroclinic orbits are generated tangent to these special equilibria’s unstable directions.

- Check first the finite equilibria, then the infinite ones.
Projective space

- One-to-one mapping of the composition space, $\mathbb{R}^R \rightarrow \mathbb{R}^R$, 

  $$
  Z_k = \frac{1}{z_k}, \quad k \in \{1, \ldots, R\},
  $$

  $$
  Z_i = \frac{z_i}{z_k}, \quad i \neq k, \quad i = 1, \ldots, R.
  $$

- This maps equilibria located at infinity into a finite domain.

- To deal with the time singularity, we add the transformation

  $$
  \frac{dt}{d\tau} = (Z_k)^{d-1},
  $$

  where $d$ is the highest polynomial degree of $f(z)$.  

Computational strategy

- We use the Bertini\textsuperscript{a} software (based on a homotopy continuation numerical technique) to compute the system’s equilibria up to any desired accuracy.

- Thermodynamic data is obtained from Chemkin-II.

- The SIM heteroclinic orbits are obtained by numerical integration of the species evolution equations using a computationally inexpensive scheme.

- Computation time is typically less than 1 minute on a 2.16 GHz MacBook Pro machine.

\textsuperscript{a}D. J. Bates, J. D. Hauenstein, A. J. Sommese, and C. W. Wampler, Bertini: Software for numerical algebraic geometry. Available at: www.nd.edu/\textasciitilde sommese/bertini.
Zel’dovich Mechanism

- The mechanism consists of $J = 2$ bimolecular reversible reactions involving $N = 5$ species $\{NO, N, O, O_2, N_2\}$ and $L = 2$ elements $\{N, O\}$.

- $z \in \mathbb{R}^2$, so selected species are $i = \{1, 2\} = \{NO, N\}$.

- The kinetic data are adopted from Baulch et al.\(^b\)

- The system is spatially homogenous with isothermal and isochoric conditions, $T = 4000 \, K$, $V = 10^3 \, cm^3$.

- Initial number of moles of all species are $n^* = 10^{-3} \, mol$.

Reactive system evolution

![Graph showing the evolution of reactive species over time](image-url)
Dynamical system formulation

- The evolution of the system is described by:

\[
\frac{d}{dt} \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} = \begin{pmatrix} 2.51 \times 10^2 + 1.16 \times 10^7 z_2 + 6.99 \times 10^8 z_2^2 \\ -9.98 \times 10^4 z_1 - 3.22 \times 10^9 z_2 z_1 \\ 2.51 \times 10^2 - 1.17 \times 10^7 z_2 - 6.98 \times 10^8 z_2^2 \\ +8.47 \times 10^4 z_1 - 1.84 \times 10^9 z_2 z_1 \end{pmatrix} \equiv f(z).}

- Employ the projective space mapping with \( d = 2 \) and \( k = 1 \):

\[
\frac{d}{d\tau} \begin{pmatrix} t \\ Z_1 \\ Z_2 \end{pmatrix} = Z_1^2 \cdot \begin{pmatrix} Z_1^{-1} \\ -Z_1 f_1 (Z_1, Z_2) \\ f_2 (Z_1, Z_2) - Z_2 f_1 (Z_1, Z_2) \end{pmatrix} \equiv F(Z),
\]
# System's equilibria

### finite

\[
R_1 \equiv (z^e) = (-1.78 \times 10^{-5}, -1.67 \times 10^{-2}) \text{ mol/g,}
\]
\[
(\lambda) = (4.18 \times 10^7, 2.35 \times 10^7) \text{ 1/s,}
\]

\[
R_2 \equiv (z^e) = (-4.20 \times 10^{-3}, -2.66 \times 10^{-5}) \text{ mol/g,}
\]
\[
(\lambda) = (-4.64 \times 10^6, 7.11 \times 10^5) \text{ 1/s,}
\]

\[
R_3 \equiv (z^e) = (3.05 \times 10^{-3}, 2.94 \times 10^{-5}) \text{ mol/g,}
\]
\[
(\lambda) = (-1.73 \times 10^7, -1.91 \times 10^5) \text{ 1/s.}
\]

### infinite

\[
I_1 \equiv (Z^e) = (0, 0),
\]
\[
(\lambda) = (-1.84 \times 10^9, 0) \text{ g/mol/s}^2,
\]

\[
I_2 \equiv (Z^e) = (0, 1.01),
\]
\[
(\lambda) = (2.54 \times 10^9, 1.12 \times 10^9) \text{ g/mol/s}^2,
\]

\[
I_3 \equiv (Z^e) = (0, 2.60),
\]
\[
(\lambda) = (3.65 \times 10^9, -2.90 \times 10^9) \text{ g/mol/s}^2.
\]
The system's 1-D SIM

\[ z \text{ mol/g} \]

\[ R \text{ mol/g} \]

\[ z_1 \text{ [mol/g]} \]

\[ z_2 \text{ [mol/g]} \]

\[ \times 10^2 \]

\[ \times 10^{-2} \]

Points: \( R_1, R_2, R_3 \)
Detailed Hydrogen-Air Mechanism

• Mechanism: \( J = 19 \) reversible reactions involving \( N = 9 \) species and \( L = 3 \) elements. \( R = 6 \), so that \( z \in \mathbb{R}^6 \).

• Kinetic model from Miller et al.\(^c\)

• Closed and spatially homogenous system with isothermal and isochoric conditions at \( T = 1500 \) \( K \), and \( V = 10^{-3} \) \( cm^3 \).

• Stoichiometric mixture \( 2H_2 + (O_2 + 3.76N_2) \).

• Selected species:

\[
i = \{1, 2, 3, 4, 5, 6\} = \{H_2, O_2, H, O, OH, H_2O\}.
\]

Reactive system evolution

\[
\begin{align*}
\text{t} & \quad \text{s} \\
10^{-5} & \\
10^{-3} & \\
10^{-7} & \\
10^{-9} & \\
\end{align*}
\]

\[
\begin{align*}
\text{n}_i & \quad \text{[mol]} \\
10^{-2} & \\
10^{-5} & \\
10^{-8} & \\
10^{-11} & \\
10^{-14} & \\
10^{-17} & \\
\end{align*}
\]

\[
\begin{align*}
\text{O}_2 & \\
\text{H}_2 & \\
\text{H}_2\text{O} & \\
\text{OH} & \\
\text{H}_2\text{O}_2 & \\
\text{O} & \\
\end{align*}
\]
System’s equilibria

- The system has 284 finite and 42 infinite equilibria.
- The set of finite equilibria contains 90 real and 186 complex 0-\(D\), one 1-\(D\), one 2-\(D\), and six 3-\(D\) equilibria.
- The set of infinite equilibria contains 18 real and 18 complex 0-\(D\), and six 1-\(D\) equilibria.
- Only 14 critical points have an eigenvalue spectrum that contains only one unstable mode.
- Inside the physical domain there is a unique equilibrium:

\[
R_{19} = (1.98 \times 10^{-6}, 9.00 \times 10^{-7}, 1.72 \times 10^{-9}, 2.67 \times 10^{-10}, 3.66 \times 10^{-7}, 1.44 \times 10^{-2}) \text{ mol/g}.
\]
3-D projection of the system’s SIM
Summary and Conclusions

• Once the difficult task of identifying all equilibria is complete, constructing the actual SIM is computationally efficient and algorithmically easy; thus, there is no need to identify it only approximately.

• Identifying all critical points, finite and infinite, plays a major role in the construction of the SIM.

• The construction procedure can be systematically extended to construct higher-dimensional SIMs.